Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Plasticity induced phase transformation in molecular crystals

Koslowski, Marisol, marisol@purdue.edu, Purdue

ABSTRACT

Solid state amorphization (SSA) can be achieved in crystalline materials including metal alloys, intermetallics, semiconductors, minerals and molecular crystals. Even though the mechanisms may differ in different materials, the crystalline to amorphous transformation occurs when the crystal reaches a metastable state in which its free energy is higher than that of the amorphous phase. SSA is observed in metal alloys because of interdiffusion of the crystalline elements during mechanical milling, thermal reaction of vapor deposited thin metal layers, mixture of metal powders and flat rolling of alternating thin metal sheets, and hydrogen reaction. We investigate the process of mechanically induced amorphization in small molecule organic crystals under extensive deformation.In this study we develop a model that describes the amorphization of molecular crystals in which plastic strain is calculated with a phase field dislocation dynamics theory in four materials: Acetaminophen, Sucrose, γ-Indomethacin, and Aspirin. The model is able to predict the fraction of amorphous material generated in single crystals for a given applied stress. Our results show that γ-Indomethacin and Sucrose demonstrate large volume fractions of amorphous material after sufficient plastic deformation, whereas smaller amorphous volume fractions are predicted in Acetaminophen and Aspirin, in agreement with experimental observation.